Indian J. Phys. **69A** (1), 163 – 168 (1995)

I J P A
- an international journal

Correlated disorder induced extended states in one dimensional lattices

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Abstract : The role of correlated disorder in producing extended electronic states in quasiperiodic and aperiodic systems is discussed. The standard picture that has emerged over the past few years is that dimer type correlations and its generalisation is responsible for the extended states in quasiperiodic copper-mean and period-doubling chains. On the other hand a new type of correlated disorder is found to be responsible for the appearance of extended electronic states in aperiodic systems like the Thue-Morse lattice. We analyse both the situations and present numerical results for the Thue-Morse chain.

Keywords : Extended states, disorder, quasiperiodicity

PACS numbers : 64.60.Ak, 71.27.+a

By now, there have been extensive discussions in the literature [1-3] on one dimensional systems lacking periodicity which show evidence of extended electronic states. The underlying cause for the appearance of extended states in such cases has been traced to the existence of a certain type of short range clustering effect among the atoms, first pointed out by Dunlap et al. [1] in their study of a distribution of random dimers on a host lattice. It was shown that at a certain energy value the composite transfer matrix for a dimer offers identity contribution to the full transfer matrix, so that at this energy the entire lattice effectively behaves as an

ordered chain. These correlations have later been shown to persist at all length scales in several quasiperiodic lattices like the copper mean chain and the period doubling lattice [2], leading to whole hierarchies of extended states.

The central feature in all the above cases is the existence of a certain cluster of atoms in the chain at every length scale, the cluster itself consisting of a repetition of a certain subcluster a finite number of times. The electronic properties for the complete chain is determined by the full transfer matrix which then has the following structure :

$$T = \ldots PPPRPRPPR \ldots$$

where R is the composite transfer matrix having itself the form M^m, where M is the transfer matrix of a subcluster, m repetitions of which generates a cluster with transfer matrix R. Here we assume that the chain is being described by the usual tight binding Anderson hamiltonian with site energies ϵ and hopping matrix elements t arrayed in accordance with the underlying quasiperiodicity of the lattice. The amplitude of the wavefunction at the nth and $(n+1)$th sites are related to those at the 0th and 1st site by the relation $\Psi_n = T\Psi_0$, where Ψ_n is a column vector consisting of the amplitudes ψ_{n+1} and ψ_n.

The appearance of extended states in such a lattice is dependent on a) the possibility of the cluster matrix R becoming equal to the identity matrix at some energy so that at these energies these clusters may be effectively disregarded and b) the possibility of the remainder of the lattice described by the transfer matrices P forming a periodic chain. Here we shall be concerned with an analysis of a) only, since in both copper-mean chain as well as the period doubling lattice the other condition b) automatically obtains [see ref.[2] for further details].

It turns out that in all cases of interest the matrix M is a 2×2 unimodular matrix, so that we may apply a well-known theorem due to Cayley and Hamilton

$$M^m = U_{m-1}(x)M - U_{m-2}(x)I \quad .$$

where $x = (1/2)TrM$, and $U_m(x) = \sin(m+1)\theta / \sin\theta$, with $\cos\theta = x$. Here $U_m(x)$ is the mth order Chebyshev polynomial of the second kind. For values of energy corresponding to the roots of the equation $U_{m-1}(x) = 0$, we effectively have M^m proportional to I, so that the

composite transfer matrix R effectively contributes only a phase factor to the full transmission. Thus if the remaining lattice forms a periodic lattice consisting of the matrices P, and the energies obtained as solutions of $U_{m-1}(x) = 0$ happen to be within the allowed band of this lattice,then the energies automatically correspond to extended states.

While many of the quasiperiodic lattices support extended states with the above type of correlated disorder as the underlying cause, there are other instances of aperiodic chains where the correlated disorder manisfests itself in an entirely different way. An example of this is the Thue-Morse chain. In this chain there is numerical evidence of extended states [4] although there is no short range dimer-type positional correlations. As we shall see, another kind of clustering effect shows up in this lattice, which cannot be analysed by the standard method outlined above and developed in detail in ref.[1,2].

A Thue-Morse (TM) chain may be built up by starting with two letters A and B and using the inflation rule $A \rightarrow AB$ and $B \rightarrow BA$ repeatedly, where the letters A and B may be thought of as representing the atoms A and B. The ratio of the numbers of A and B atoms in any generation ℓ is $N_A(\ell)/N_B(\ell) = 1$. We again use the tight-binding one-band hamiltonian to describe this sytem, and for convenience we set the hopping integral equal to unity.

As before, the amplitude of the wave function at the n-th site is related to that at the first site by the following matrix product

$$M_n M_{n-1} \cdots\cdots\cdots M_1 \ .$$

where M_n is the transfer matrix for a single atom.

In order to unravel the correlations that are responsible for the extended states in a Thue-Morse chain, we first recapitulate the structural peculiarities of this lattice. At the very basic level, we may regard the atoms A and B to be the basic building blocks of the TM lattice; at the next level the pairs AB and BA may be regarded as the basic starting elements on which the repeated application of the Thue-Morse inflation rules generates the whole lattice. We may successively consider the pair of quadruplets $ABBA$ and $BAAB$, the pair $ABBABAAB$ and $BAABABBA$, the pair $ABBABAABBAABABBA$ and $BAABABBAABBABAAB$ etc. as the starting blocks for generating the Thue-Morse chain by applying the appropriate inflation rules.

Evidently, there are no dimer or higher order atomic clustering in this lattice. It thus becomes necessary to analyse the products of transfer matrices corresponding to these strings of atoms in order to understand the conditions under which extended states are supported by the TM lattice.

To handle such long products of matrices we resort to the following device. Let us begin by resolving the 2×2 matrices M_n in a basis formed by the 2×2 identity matrix I and the three Pauli matrices σ_x, σ_y and σ_z. We then have the expressions for M_A and M_B in the following form:

$$M_A = \alpha_A I + \beta_A \sigma_x + \gamma_A \sigma_y + \delta_A \sigma_z$$

$$M_B = \alpha_B I + \beta_B \sigma_x + \gamma_B \sigma_y + \delta_B \sigma_z$$

where $\alpha_{A(B)} = \delta_{A(B)} = (E - \epsilon_{A(B)})/2$, $\beta_{A(B)} = 0$ and $\gamma_{A(B)} = -i$.

Using this equation repeatedly, we can easily find the forms of the longer matrix products mentioned above. Interestingly, the pair of products of matrices $M_A M_B M_B M_A M_B M_A M_A M_B \ldots$ and $M_B M_A M_A M_B M_A M_B M_B M_A \ldots$ each with 2^n elements show a surprising regularity having either of the following forms

$$\begin{aligned} M_A M_B M_B M_A M_B M_A M_A M_B \cdots &= \alpha_n I + \gamma_n \sigma_y + \delta_n \sigma_z \\ M_B M_A M_A M_B M_A M_B M_B M_A \cdots &= \alpha_n I + \gamma_n' \sigma_y + \delta_n' \sigma_z \end{aligned} \qquad (n \text{ even})$$

and

$$\begin{aligned} M_A M_B M_B M_A M_B M_A M_A M_B \cdots &= \alpha_n I + \beta_n \sigma_x + \gamma_n \sigma_y + \delta_n \sigma_z \\ M_B M_A M_A M_B M_A M_B M_B M_A \cdots &= \alpha_n I - \beta_n \sigma_x + \gamma_n \sigma_y + \delta_n \sigma_z \end{aligned} \qquad (n \text{ odd}).$$

It follows that the matrix products $M_A M_B M_B M_A M_B M_A M_A M_B \cdots$ and $M_B M_A M_A M_B M_A M_B M_B M_A \cdots$ can never be made equal at some value of the energy for even values of n because their expansions differ in two coefficients γ and δ. On the other hand, for odd values of n, the above equations show that the matrix products become equal to each other if $\beta_n = 0$. Thus the energy values for which $\beta_n = 0$ (n odd) are the ones for which the composite transfer matrices for of the strings of atoms $ABBABAAB \cdots$ and $BAABABBA \cdots$ offer identical

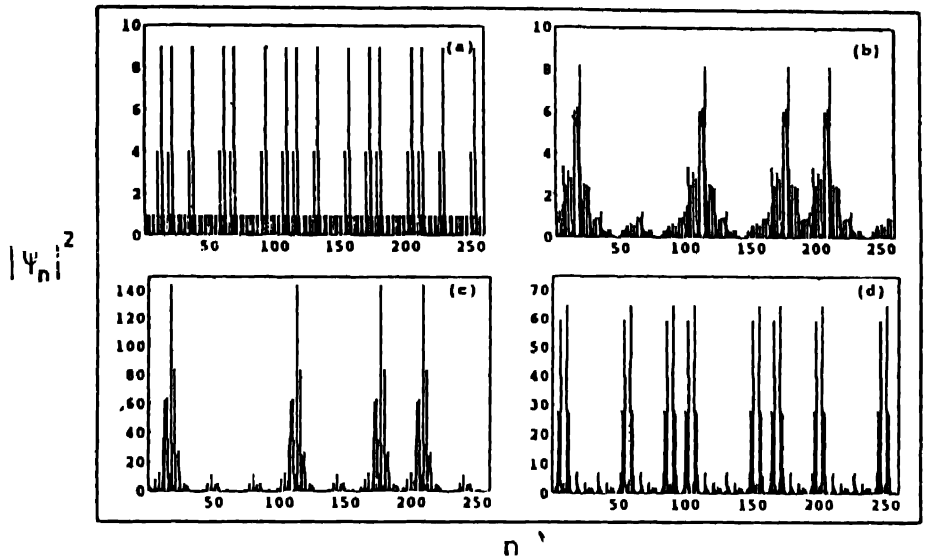

Fig.1 Plot of $|\psi_n|^2$ versus site number n for a TM sequence with 256 sites. Here $\epsilon_A = -\epsilon_B = 0.5$ with energies measured in units of hopping matrix element t. Figs.(a), (b), (c) and (d) correspond respectively to energies 1.5,0.337965671230,−1.260097834748 and −1.995507972823.

contributions to the full transfer matrix for the whole chain. Since the Thue-Morse chain may be regarded as built out of these composite blocks, the full transfer matrix for the whole chain now consists of a product of identical unimodular 2×2 matrices M, each corresponding to a block of atoms $ABBABAAB\cdots$ or $BAABABBA\cdots$.

The recursion relations connecting the α, β, γ and δ between successive generations may be found after some algebra, and it is straighforward to obtain the algebraic expressions for the energy values obtained from the condition $\beta_n = 0$. For the sake of illustration we display in Fig.1 the variation of $|\psi|^2$ with the site-index n for a few selected energies. The signature of the underlying Thue-Morse aperiodicity is particularly apparent in Figs.1(a), 1(c) and 1(d); all the wave-functions are lattice-like. The general characteristic of these functions is that with increasing n, amplitudes tend to cluster around groups of sites separated by islands where the amplitudes have very low values, a fact which was also pointed out by Ryu et al. [5].

The spirit in which the present analysis has been carried out corresponds to the real space renormalisation group point of view. Here the renormalisation process becomes evident when we resolve the composite matrices in the basis of the Pauli matrices, a resolution which clearly reveals the repeating character of the strings of matrices in alternate generations.

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